

Microsymposium

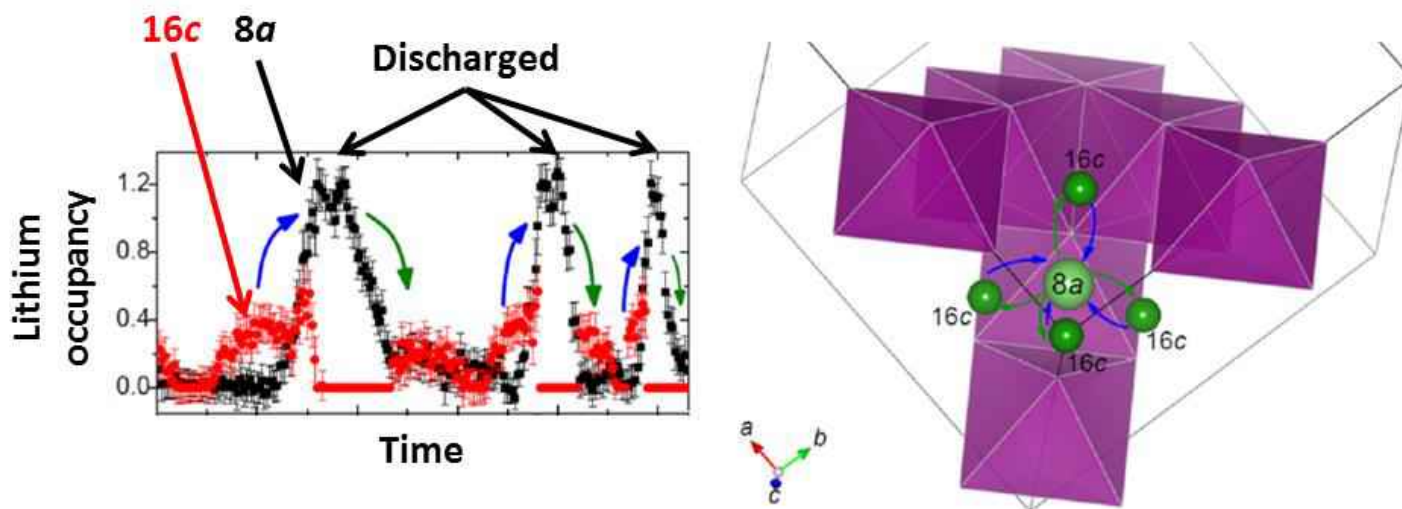
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Time-resolved in situ neutron diffraction studies of Li-ion battery materials

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Lithium-ion batteries are ubiquitous in society, used in everything from children's toys to mobile electronic devices, providing portable power solutions. There is a continuous drive for the improvement of these batteries to meet the demands of higher power devices and uses. A large proportion of the function of lithium-ion batteries arises from the electrodes, and these are in turn mediated by the atomic-scale perturbations or changes in the crystal structure during an electrochemical process (e.g. battery use). Therefore, a method to both understand battery function and propose ideas to improve their performance is to probe the electrode crystal structure evolution in situ while an electrochemical process is occurring inside a battery. Our work has utilized the benefits of in situ neutron diffraction (e.g. sensitivity towards lithium) to literally track the time-resolved evolution of lithium in electrode materials used in lithium-ion batteries (see Figure 1). With this knowledge we have been able to directly relate electrochemical properties such as capacity and differences in charge/discharge behaviour of a battery to the content and distribution of lithium in the electrode crystal structure. This talk will showcase some of our in situ investigations of materials in lithium-ion batteries, such as LiCoO_2 , LiFePO_4 , $\text{Li}_{1+y}\text{Mn}_2\text{O}_4$, $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{Li}_4\text{Ti}_5\text{O}_{12}/\text{TiO}_2$ electrodes. In addition, selected examples of our work using time-resolved in situ X-ray diffraction to probe other batteries types, such as primary lithium and secondary (rechargeable) sodium-ion batteries will be presented. Using time-resolved diffraction data, a comprehensive atomic-scale picture of battery functionality can be modelled and permutations can be made to the electrodes and electrochemical conditions to optimize battery performance. Therefore, crystallography and electrochemistry can mesh together to solve our energy needs.



Keywords: In-situ experimentation, electrodes, insertion/extraction reactions